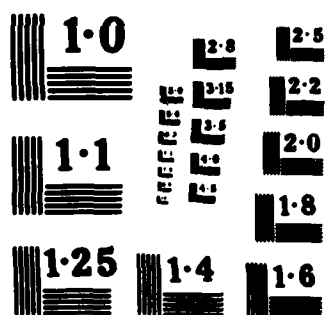


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TRANSPORT PROPERTIES AND DISTRIBUTION FUNCTIONS  
IN III - V SEMICONDUCTORS

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November, 1984

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FIELD	GROUP	SUB. GR.		
19. ABSTRACT (Continue on reverse if necessary and identify by block number) Approximate analytical expressions for electron distribution functions in III-V semiconductors have been derived for high and low electric fields. For low electric fields two analytic methods were used and compared with an earlier iteration method and a new perturbation method. All gave similar distribution functions and drift mobility. For high electric fields the electron distribution function was found within the diffusion approximation by an expansion inversely in the electric field. For $Al_{0.25}In_{0.75}$ As the effects of p-wave scattering and nonparabolic energy bands were not found to be the cause of the negative differential resistance. Alloy scattering in ternary semiconductors was treated in the coherent potential approximation. The validity of the diffusion and maximum anisotropy approximation has been assessed by an expansion inversely in the electric field of the polar optical collision term in high electric fields.				
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## I. OBJECTIVES OF RESEARCH

The objective of this research was to derive approximate analytic expressions for electron distribution functions in III-V semiconductors in order to calculate transport properties. The approach was viewed as an alternative to Monte Carlo and drifted Maxwellian calculations. The use of analytic expressions for the electron distribution function was intended to reduce the cost of numerical calculations and to facilitate parameter studies of transport coefficients, in particular the temperature dependence of the drift mobility. The objective during the two years of this contract was to focus on the high electric field regime for GaAs, InP and ternary semiconductors such as  $\text{Al}_{0.25}\text{In}_{0.75}\text{As}$ . For ternary III-V semiconductors nonparabolic energy bands were to be included in the central valley for polar optical scattering in order to understand the negative differential resistance predicted for electrons in the central valley alone. Alloy scattering was also to be considered. An attempt to include intervalley scattering for GaAs was to be made. All new results were to be compared with previous numerical and experimental results where possible.

## II. SUMMARY OF RESEARCH RESULTS

Several related research topics have been explored. The main thrust of the research has been the development of theoretical methods for calculating electron distribution functions and the drift mobility in III-V semiconductors. The contract has supported in addition to the principal investigator one graduate student, Sik Han Soh, who completed his master's thesis in August, 1984. He is now employed as a project engineer working with III-V semiconductors at Hewlett-Packard in Singapore. His thesis<sup>1</sup> was entitled "Electron Distribution Functions and Mobility in III-V Semiconductor Compounds for High and Low Electric Fields". A paper<sup>2</sup> on part of this work appears in The Physics of Submicron Structures which has been published by Plenum. A second paper is planned on the effect of p-wave scattering and nonparabolic energy bands on the negative differential resistance arising in the central valley of the conduction band for certain ternary III-V semiconductors. Also a short collaboration

with Professor Peter Fedders of the Physics Department at Washington University and Professor Charles Myles of the Physics Department at Texas Tech University on the coherent potential approximation applied to alloy scattering in ternary III-V semiconductors resulted in a talk<sup>3</sup>. For comparable percentages of disorder the scattering due to off-diagonal disorder was found to dominate in alloy scattering in a two-band model for III-V semiconductors. This project was not pursued further by the principal investigator because a subsequent paper by Professors Dan Rode and Peter Fedders<sup>4</sup> showed that for most ternary III-V semiconductors of interest in device applications the Born approximation could be justified such that the coherent potential approximation is not really needed. A resolution of some of the differences in the diffusion approximation<sup>5</sup> and the maximum anisotropy approximation<sup>6,7</sup> used to simplify the electron distribution function at high d.c. electric fields has been made by means of an asymptotic expansion inversely in the electric field of the steady-state Boltzmann equation for polar optical scattering. A better understanding of the applicability of these approximations is now feasible<sup>8</sup>. Preliminary calculations on the extension of the calculation of the electron distribution function by approximate analytic expressions for intervalley scattering was begun. That effort was not continued because of an uncertainty in the basis of the validity of the diffusion and maximum anisotropy approximations and because the principal investigator ran out of time in one year. The drift mobility for InP was calculated but not investigated further as the time-of-flight data was not available.

The master's thesis of Mr. Soh included several methods for determining electron distribution functions in low electric fields and the calculation of the electron drift mobility for polar optical scattering. The methods were: iteration<sup>9</sup>, perturbation, and two analytic methods. The iteration method was calculated numerically and compared with previous numerical results that had been compared with experimental data. The perturbation method was numerical but the two analytic

methods produced approximate analytic expressions for the electron distribution function from which the drift mobility was calculated. The results from all methods were similar. For high electric fields the expansion of the steady-state Boltzmann equation inversely in the electric field within the diffusion approximation for the electron distribution function was reviewed<sup>2</sup>. The electron distribution function was compared with that derived by Stratton<sup>10</sup> for parabolic energy bands and agreement found for an expansion in  $1/E$  of his result. Neither distribution function is normalizable and intervalley scattering needs to be included for GaAs; for certain ternary III-V semiconductors intervalley scattering may be omitted in a certain range. For high electric fields p-wave scattering and nonparabolic energy bands were included in the polar optical scattering term. For GaAs and even  $\text{Al}_{0.25}\text{In}_{0.75}\text{As}$  the effects of p-wave scattering and nonparabolic energy bands were not found to alter the electron distribution significantly. Consequently the negative differential resistance for ternary III-V semiconductors does not appear to be caused by the nonparabolic character of the central valley of the conduction band. Another supporting argument for our conclusion can be found in the Monte Carlo calculations<sup>11</sup> of the electron drift velocity-electric field curve where p-wave scattering is negligible. As Rode<sup>12</sup> has pointed out nonparabolic energy bands exist only if there are p-wave matrix elements as well as s-wave matrix elements. Hence, one cannot invoke nonparabolic energy bands at the same time p-wave scattering is dropped.

To compare the diffusion and maximum anisotropy approximations an expansion inversely in the electric field has been made of the steady-state Boltzmann equation for a d.c. electric field and polar optical scattering. This model is expected to be reasonable for ternary semiconductors if alloy scattering is added; for GaAs intervalley scattering should be added. For  $E_0/E$  small where  $E_0$ <sup>13</sup> is the critical electric field characterized by the strength of the coupling to the polar modes, the symmetric part of the distribution function for electrons in the central valley is a constant. The asymmetric part of the electron distribution function can be

represented as an expansion in odd order Legendre polynomials whose argument is the cosine of the angle between the electric field and wave vector. The coefficients of the odd order Legendre polynomials for high electric fields and electron energies high compared to an optical phonon energy obey a modified maximum anisotropy relation where no even order coefficients for  $n > 0$  exist. The diffusion approximation does not give the entire electron distribution function correctly but for high electric fields it produces a functional from which the electron density and drift velocity for electrons in the central valley can be correctly calculated for polar optical scattering.

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## PERSONNEL

Principal Investigator - Barbara Abraham-Shrauner  
Graduate Student - Sik Han Soh

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- S. H. Soh, Master's Thesis, "Electron Distribution Functions and Mobility in III-V Semiconductor Compounds for High and Low Electric Fields", Washington University in St. Louis, August, 1984.
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